Dynamic structure function of a cold Fermi gas at unitarity

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We present a theoretical study of the dynamic structure function of a resonantly interacting two-component Fermi gas at zero temperature. Our approach is based on dynamic many-body theory able to describe excitations in strongly correlated Fermi systems. The fixed-node diffusion Monte Carlo method is used to produce the ground-state correlation functions which are used as an input for the excitation theory. Our approach reproduces recent Bragg scattering data in both the density and the spin channel. In the BCS regime, the response is close to that of the ideal Fermi gas. On the BEC side, the Bose peak associated with the formation of dimers dominates the density channel of the dynamic response. When the fraction of dimers is large our theory departs from the experimental data, mainly in the spin channel.

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An impressive advance in realizing and controlling ultracold Fermi gases has permitted to study physical phenomena whose appearance was previously only a matter of speculation [1]. One of the major advances has been the first clean observation of a crossover between two limits of Fermi matter, the Bose-Einstein condensate (BEC) regime composed by Fermi molecules and the Bardeen-Cooper-Schrieffer (BCS) superfluid gas where Cooper pairs are formed [2–5].

In the dilute limit, interactions between atoms can be described by a single parameter, namely the s-wave scattering length a. The system evolves from a BCS regime with no bound state ($a < 0$) to a molecular one (BEC) with a two-body bound state ($a > 0$), crossing a singular point where $|a| \to \infty$ corresponding to a Fano-Feshbach resonance [6–8]. This special point is referred to as the unitary limit and is expected to show a number of universal properties. Indeed, in this regime the only relevant length and energy scales are the inverse Fermi momentum k_F^{-1} and the Fermi energy $E_{\rm F}$, respectively.

Nowadays, the unitary Fermi gas is routinely realized in experiments. An acccurate theoretical description of the unitary limit requires the use of advanced methods of many-body theory that can deal with strongly interacting systems. In this situation, quantum Monte Carlo methods have proven to be very useful for the calculation of the finite- and zero-temperature equation of state [6–9] which is found to be in good overall agreement with experimental data [10, 11]. Also, it was possible to predict the effect of the unbalanced population [12] and different masses [13]. More recently, static responses such as the spin susceptibility and spin diffusivity [14, 15] have been measured and also studied theoretically using quantum Monte Carlo (QMC) methods [16] and a diagrammatic approach [17].

Recently, Hoinka *et al.* [18, 19] have measured the dynamic spin and density responses of a Fermi gas at unitarity and in the BEC regime. In order to measure both responses, they used two-photon Bragg scattering, acting on ^{6}Li at very low temperature ($\sim 0.06 E_{\rm F}$ at unitarity), and a proper choice of the laser detuning. The density response at unitarity is significantly different from that of an ideal Fermi gas, showing a clear peak which corresponds to the formation of dimers composed of spin-up and spin-down particles. This signature of dimer formation is not visible in the spin channel, nevertheless our results are quite different from the ideal Fermi gas response. This provides evidence for the importance of correlations in the unitary gas despite its diluteness.

Some of the features shown by the dynamic response function at unitarity were previously determined in theoretical work: at $T = 0$ using a dynamic self-consistent mean-field approach based on BCS theory [20], at $T > 0$ using virial expansions [21]. However, the dynamic properties along the BCS-BEC crossover are not completely understood due to the need of a full many-body theory and the impossibility to use QMC methods directly. The goal of our study is to pursue further a theory for the dynamic structure function, combining the virtues of Monte Carlo methods and modern diagrammatic many-body theory.

In the present work, we study the density and spin responses of the two-component Fermi gas at unitarity and in characteristic points on both the BEC and BCS sides of the crossover. We use a fully microscopic approach utilizing correlated basis function (CBF) theory. The input ground-state structure functions are obtained from diffusion Monte Carlo simulations within the fixed-node (FN-DMC) approximation [6]. In its most advanced form [22], the dynamic many-body theory (DMBT) used here is the fermion version of the CBF-Brillouin-Wigner perturbation theory previously developed for bosons [23]. The power of DMBT for fermions has been recently demonstrated by the prediction of a stable roton excitation in

two-dimensional ^{3}He, which has independently been confirmed by inelastic neutron scattering experiments [24].

Inputs for the calculation of the dynamic response are the static structure factors, $S_{\uparrow\uparrow}(k)$ and $S_{\uparrow\downarrow}(k)$, and the fraction of dimers along the BCS-BEC crossover. We obtain a complete description of the density and spin dynamic responses in the momentum-energy plane. In the unitary limit, both theoretical responses are in satisfactory agreement with the recent experimental Bragg scattering measurements [18].

In weakly interacting systems, time-dependent Hartree-Fock (TDHF) theory [25] is a well-established method for capturing the dynamics. One assumes that the system is subjected to the perturbing Hamiltonian

$$\delta\hat{H}_{\rm ext}(t) = \int d^3r \hat{\rho}^{(\rho/\sigma)}(\mathbf{r}) h_{\rm ext}(\mathbf{r},t)\,; \tag{1}$$

the superscripts ρ and σ stand for density and spin excitations, respectively. $\hat{\rho}^{(\rho/\sigma)}(\mathbf{r})$ is the (spin-)density operator, and $h_{\rm ext}(\mathbf{r},t)$ is a weak, local external field. The wave function resulting from such a perturbation is assumed to be of the form

$$|\psi\rangle = e^{1/2\sum_{ph} c_{ph}(t) a_p^\dagger a_h}|\phi_0\rangle\,, \tag{2}$$

where $|\phi_0\rangle$ is the ground state of a non-interacting system with the same density. The particle ("p") and hole ("h") labels run over spatial quantum numbers and spin degrees of freedom.

The amplitudes $c_{ph}(t)$ are Fourier decomposed

$$c_{ph}(t) = c_{ph}^{(+)}(\omega)e^{-\imath(\omega+\imath\eta/\hbar)t} + c_{ph}^{(-)*}(\omega)e^{\imath(\omega+\imath\eta/\hbar)t}\,. \tag{3}$$

Equations of motion are then derived from a least action principle [26, 27] . They are given by

$$\big(\hbar\omega+\imath\eta-\epsilon_{ph}\big)c_{ph}^{(+)}(\omega) - \sum_{p'h'} V_{ph;p'h'}c_{p'h'}^{(+)}(\omega) - \sum_{p'h'} V_{pp'hh';0}c_{p'h'}^{(-)}(\omega) = 2\int d^3r \rho_{ph;0}^{(\rho/\sigma)}(\mathbf{r}) h_{\rm ext}(\mathbf{r},\omega) \tag{4}$$

$$\big(-\hbar\omega-\imath\eta-\epsilon_{ph}\big)c_{ph}^{(-)}(\omega) - \sum_{p'h'} V_{p'h';ph}c_{p'h'}^{(-)}(\omega) - \sum_{p'h'} V_{0;pp'hh'}c_{p'h'}^{(+)}(\omega) = 2\int d^3r \rho_{0;ph}^{(\rho/\sigma)}(\mathbf{r}) h_{\rm ext}(\mathbf{r},\omega), \tag{5}$$

where $h_{\rm ext}(\mathbf{r},\omega)$ is the Fourier component of the external field.

From the solutions $c_{ph}^{(\pm)}(\omega)$ we can calculate the (spin-) density response function

$$\chi^{(\rho/\sigma)}(\mathbf{r},\mathbf{r}',\omega) \equiv \frac{1}{\rho(\mathbf{r})\rho(\mathbf{r}')}\frac{\delta\langle\psi|\,\hat{\rho}^{(\rho/\sigma)}\,|\psi\rangle(\mathbf{r},\omega)}{\delta h_{\rm ext}(\mathbf{r}',\omega)}\,, \tag{6}$$

and the (spin-)density dynamic structure function

$$S^{(\rho/\sigma)}(\mathbf{r},\mathbf{r}',\omega) \equiv -\frac{1}{\pi}{\rm Im}\chi^{(\rho/\sigma)}(\mathbf{r},\mathbf{r}',\omega) \tag{7}$$

in coordinate space. In a translationally invariant geometry, their momentum space representations, $\chi^{(\rho/\sigma)}(q,\omega)$ and $S^{(\rho/\sigma)}(q,\omega)$, are functions of the momentum transfer q.

Key ingredients of the equations of motion are the matrix elements of the interparticle interaction

$$V_{ph;p'h'} = \langle ph'|\,V_{\rm d}\,|hp'\rangle - \langle ph'|\,V_{\rm ex}\,|p'h\rangle \tag{8}$$

$$V_{pp'hh';0} = \langle pp'|\,V_{\rm d}\,|hh'\rangle - \langle pp'|\,V_{\rm ex}\,|h'h\rangle \tag{9}$$

and the single-particle spectrum $\epsilon_{ph} = \epsilon_p - \epsilon_h$. Generally, the potentials $V_{\rm d}$ and $V_{\rm ex}$ are effective interactions in the direct and exchange channel, respectively. In conventional TDHF theory, they are the same and just the bare interaction between the particles. The ϵ_p, ϵ_h are the Hartree-Fock single-particle energies. Using the CBF method, the description can be extended to strongly interacting systems [28, 29]. The basic outcome of the rather intricate diagrammatic analysis is that one arrives at the same equations of motion. CBF theory provides a method for computing effective interactions from the bare interaction. These interactions are normally different in the direct and the exchange channels.

If one neglects exchange effects, one can construct $V_{\rm d}$ from the static structure function by demanding that $V_{\rm d}$ reproduces $S^{(\rho)}(q)$ through the ω^0 sum rule

$$S^{(\rho)}(q) = \int_0^\infty d(\hbar\omega) S^{(\rho)}(q,\omega)\,. \tag{10}$$

A useful analytic relationship which is accurate within one to two percent can be derived using a collective approximation for the Lindhard function,

$$V_{\rm d}(q) = \frac{\hbar^2q^2}{4m}\Big(\frac{1}{S^{(\rho)}(q)^2} - \frac{1}{S_{\rm F}(q)^2}\Big)\,, \tag{11}$$

where $S_{\rm F}(q)$ is the static structure factor of the free Fermi gas.

For spin-independent interactions, the spin-density fluctuations depend on $V_{\rm ex}(q)$ but not on $V_{\rm d}(q)$. Thus one might be tempted to construct $V_{\rm ex}(q)$ from $S^{(\sigma)}(q)$ in a

similar fashion as $V_{\rm d}(q)$ is derived from $S^{(\rho)}(q)$. Unfortunately, this procedure has numerical difficulties because the resulting problem is very poorly conditioned. We therefore utilize an expression obtained from the Fermi-Hypernetted-Chain (FHNC) analysis which suggests, in its simplest form [30], a local exchange interaction

$$V_{\rm ex}(q) = -\frac{\hbar^2 q^2}{2m}\,\frac{S^{(\rho)}(q) - S_{\rm F}(q)}{S_{\rm F}(q)^3}\,. \qquad (12)$$

The same effective interaction defines the single-particle spectrum

$$\epsilon_k = \frac{\hbar^2 k^2}{2m} - \frac{1}{\nu N}\sum_h V_{\rm ex}(|\mathbf{k}-\mathbf{h}|)\,, \qquad (13)$$

where ν is the spin degeneracy and N the number of particles. A consistent treatment of the exchange potential and the single particle spectrum is needed to satisfy the ω^1 sum rule.

The calculation of the potentials $V_{\rm d}(q)$ (11) and $V_{\rm ex}(q)$ (12) requires knowledge of no more than the density structure function of the interacting system, $S^{(\rho)}(q)$. For that, we use ground-state results obtained using the FN-DMC method [6], which has proven its accuracy in the description of the BCS-BEC crossover.

We have calculated the dynamic structure function in the density and spin channels for $1/(k_{\rm F}a) = -1$ (BCS like), $1/(k_{\rm F}a) = 0$ (unitarity) and $1/(k_{\rm F}a) = 1$ (BEC like) including exchange terms and non-local, energy-dependent CBF corrections that are not spelled out explicitly, see Ref. [29]. Paying attention to the fact that, with decreasing $1/(k_{\rm F}a)$, the system favors the creation of bound dimers, we consider a non-interacting mixture of dimers ("bosons" with $2m$) and atoms (fermions). The relative concentrations by which we weight the two contributions to the dynamic structure function in the density channel are obtained from our FN-DMC ground-state calculations. In particular, the concentration of dimers as a function of the scattering length is estimated assuming that all pairs are in the zero-momentum state. According to this criterion, the concentration of dimers is 100% deep inside the BEC regime and decreases to zero quickly after crossing the unitary limit where it amounts $\sim 50\%$ [31]. Our model cannot predict the width of the "Bose" peak, hence it has been fitted to reproduce the width of the experimental data subject to the constraint that its contribution to the ω^0 sum rule is constant. The spin channel dynamics on the other hand is not affected by the presence of dimers because they do not contribute to spin-density fluctuations.

In Fig. 1, we show results of $S^{(\rho)}(k,\omega)$ and $S^{(\sigma)}(k,\omega)$ for the wave vector $q = 4.5\,k_{\rm F}$. We have selected this particular q value because it is the only momentum measured by Bragg scattering [18]. In agreement with the experimental data, the density channel of the dynamic

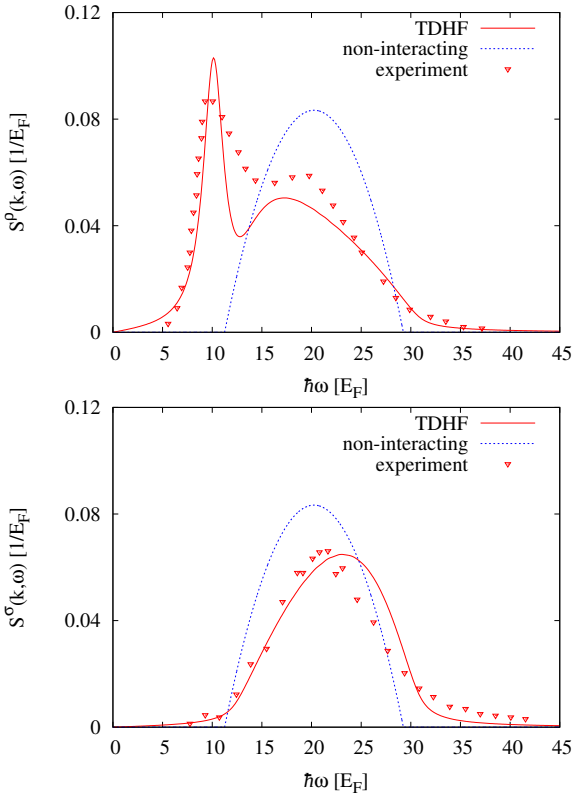

FIG. 1. (Color online) The dynamic structure function in the density (*top*) and spin (*bottom*) channels at unitarity ($1/(k_F a) = 0$) and at a momentum $q = 4.5k_{\rm F}$ (solid line). The points are the experimental data of Ref. [18]. Dashed line stands for the non-interacting response.

structure function shows a clear "Bose" peak centered at energy $\hbar^2k^2/4m$ coming from the scattering off the ↑-↓ pairs. At higher energies, contribution of single Fermi atoms appear as a broader response. The importance of correlations at unitarity is best demonstrated by comparing the response coming from the full theory with the non-interacting Lindhard function, also shown in Fig. 1. Our result for the spin channel at unitarity and the same q value as in the experiment is also shown in Fig. 1 (bottom panel). As mentioned above, dimers do not contribute to the spin channel and only atomic contributions appear. As in the density channel, the use of many-body theory is crucial to describe the experimental data, note that the response of a non-interacting system has a completely different structure and differs substantially from what was observed in the experiment.

The full momentum-energy dependence of the density and spin response functions is shown as density plots in Fig. 2. At low momenta, $k \lesssim 4k_F$, the dimer peak lies inside the particle-hole ($p-h$) band and has a large overlap with the single-atom scattering contribution. At higher momenta, the "Bose" peak is progressively decoupled of Fermi excitations with a position given by half the recoil

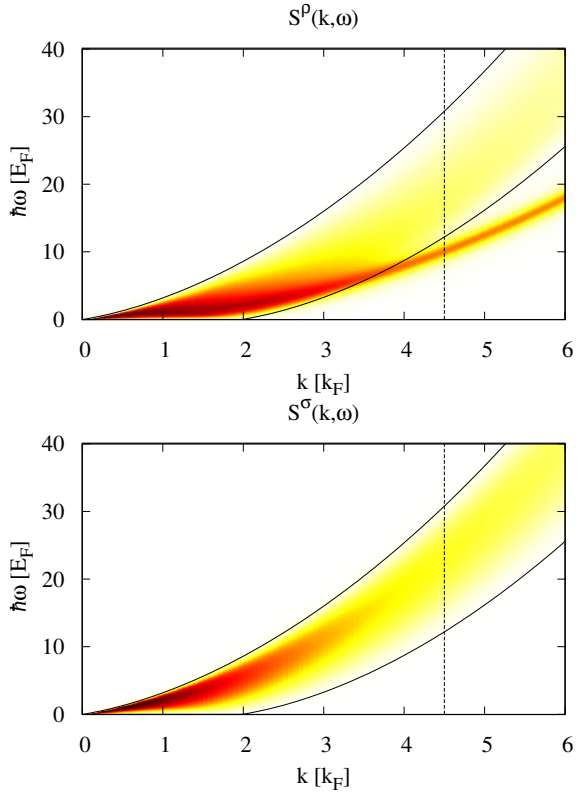

FIG. 2. (Color online) The dynamic structure function in the density (*top*) and spin (*bottom*) channels at unitarity ($1/(k_F a) = 0$) as a function of the momentum transfer k and energy transfer $\hbar\omega$ in units of the Fermi energy E_F. The solid lines show the limits of the particle-hole band. The vertical dashed line corresponds to the momentum transfer at which the experiment of Ref. [18] was performed.

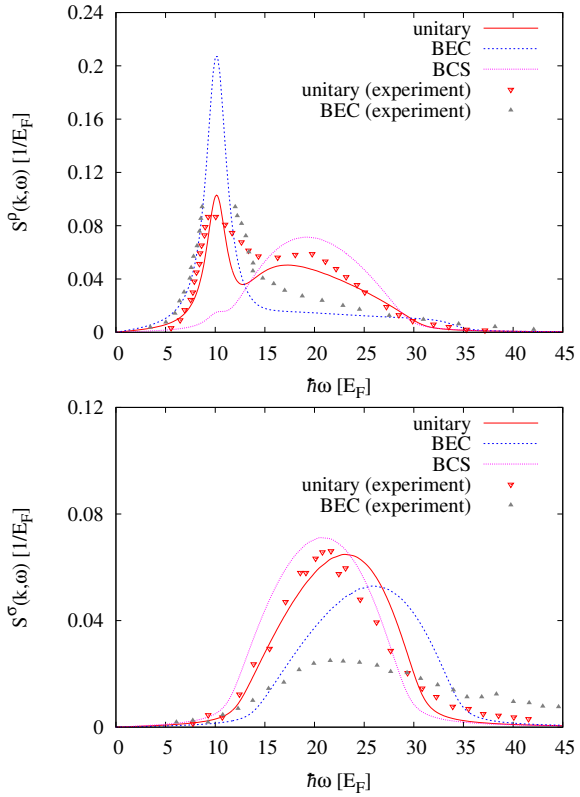

FIG. 3. (Color online) The dynamic structure function in the density (*top*) and spin (*bottom*) channels at unitarity ($1/(k_F a) = 0$), BEC ($1/(k_F a) = 1$), and BCS ($1/(k_F a) = -1$). The lines are results from dynamic many-body theory and points are experimental data of Ref. 18. All data corresponds to $q = 4.5 k_F$.

energy. The strength of the spin response is localized inside the $p-h$ band but interactions make the peak slightly asymmetric and shifted to higher energy compared with the non-interacting response; this effect is washed out at momenta $k \gtrsim 4k_F$.

Bragg scattering [18, 19] was also applied to a point in the phase diagram located in the BEC side, in particular at $1/(k_F a) = 1$, whereas no experimental data exists in the BCS side. We have applied dynamic many-body theory to the experimental BEC point and to the symmetric one in the BCS side, with $1/(k_F a) = -1$, and at a momentum transfer $q = 4.5 k_F$. The response in the BCS regime is rather close to that of the free Fermi gas, with only an incipient Bose peak from the dimer contribution due to its very low concentration (< 10 %). On the contrary, the dimer contribution dominates the density channel in the BEC side since the concentration of dimers is ~ 90 %. Our theory, which produces results in good agreement with experiment in the unitary limit, seems to worsen in the BEC regime. This is seen most clearly in the spin response at $1/(k_F a) = 1$ where our result does not show the broad response obtained from Bragg scattering.

To conclude, motivated by the first measurements of the dynamic structure function of a two-component resonantly interacting Fermi mixture, we have developed a theory able to predict its dynamic response. To this end, dynamic many-body theory is used together with a FN-DMC input for the static structure factor. From a direct comparison with experimental data [18], we show that the ideal Fermi gas model is not sufficient to reproduce correctly the dynamic response functions. We have formulated a description in terms of a mixture of dimers (bosons) and atoms (fermions). This simple model permits to capture correctly the complicated structure of the density response at the unitary limit. Our theory departs from the experimental data, mainly in the spin channel, when the fraction of dimers is large. Finally, we provide information on the dynamic response for different (previously not measured) values of the momentum in the unitary limit and on the BCS (not measured) side.

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